For general semiconductors, you can use Equations 3-59 and 3-60 without the transitions to complete ionization. To enable this model, specify INC.ION in the MODEL statement.

3.3.2 Low Temperature Simulations

In conjunction with Fermi-Dirac statistics and impurity freeze-out, ATLAS simulates device behavior under low operating temperatures. In general, simulations can be performed at temperatures as low as 50K without loss of quadratic convergence. Below this temperature, carrier and ionization statistics develop sharp transitions which cause slower convergence. Since many more iterations will probably be required if temperatures below 50K are specified, the ITLIMIT parameter of the METHOD statement should be increased.

Due to the limited exponent range on some machines, ATLAS can have trouble calculating the quasi-Fermi level of minority carriers. As the temperature decreases, the intrinsic carrier concentration also decreases. In quasi-neutral regions, the minority carrier concentration can easily underflow. Such situations were handled in the past by setting these concentrations to zero. This method does not allow an accurate subsequent calculation of minority carrier quasi-Fermi levels. In order to accurately calculate quasi-Fermi levels, majority carrier concentration and the relation, $np=n_{ie}^2$ is used to obtain minority carrier concentrations in case of an underflow. Despite these efforts, spurious glitches are occasionally observed at low temperatures in the minority quasi-Fermi levels.

3.3.3 Traps and Defects

Semiconductor materials exhibit crystal flaws, which can be caused by dangling bonds at interfaces or by the presence of impurities in the substrate. The presence of these defect centers, or traps, in semiconductor substrates may significantly influence the electrical characteristics of the device. Trap centers, whose associated energy lies in a forbidden gap, exchange charge with the conduction and valence bands through the emission and capture of electrons. The trap centers influence the density of space charge in semiconductor bulk and the recombination statistics.

Device physics has established the existence of three different mechanisms, which add to the space charge term in Poissons's equation in addition to the ionized donor and acceptor impurities. These are interface fixed charge, interface trap states and bulk trap states. Interface fixed charge is modeled as a sheet of charge at the interface and therefore is controlled by the interface boundary condition. Interface traps and bulk traps will add space charge directly into the right hand side of Poisson's equation. This section describes the definition of bulk trap states and the implementation of these bulk trap states into ATLAS for both steady state and transient conditions.

A donor-type trap can be either positive or neutral like a donor dopant. An acceptor-type trap can be either negative or neutral like an acceptor dopant. A donor-like trap is positively charged (ionized) when empty and neutral when filled (with an electron). An empty donor-type trap, which is positive, can capture an electron or emit a hole. A filled donor-type trap, which is neutral, can emit an electron or capture a hole. An acceptor-like trap is neutral when empty and negatively charged (ionized) when filled (with an electron). A filled acceptor-like trap can emit an electron or capture a hole. An empty acceptor-like trap can capture an electron or emit a hole. Unlike donors, donor-like traps usually lie near the valence band. Likewise, acceptor-like traps usually lie near the conduction band.

Figure 3-1 shows the terminology used within ATLAS to define the type of trap. The position of the trap is defined relative to the conduction or valence bands using E.LEVEL so for instance, an acceptor trap at 0.4eV would be 0.4eV below the conduction band.

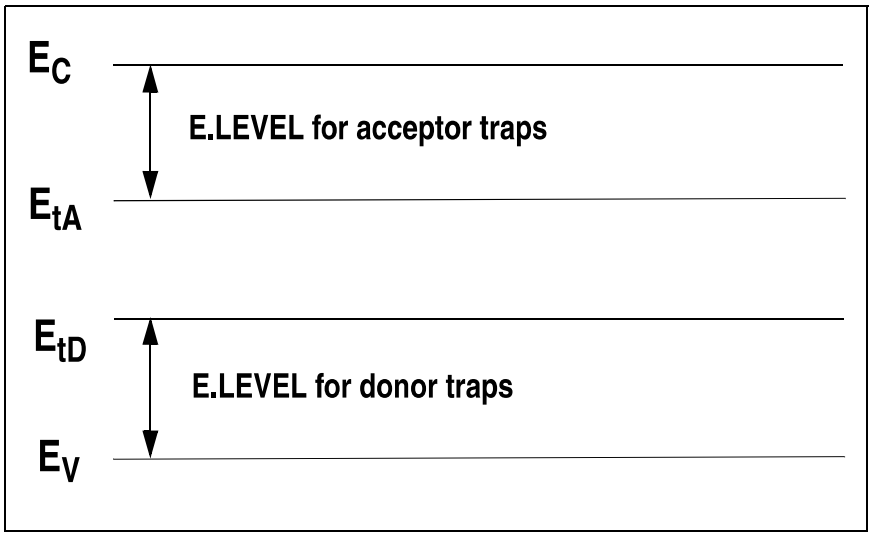

Figure 3-1: Definition of the trap energy level for acceptor and donor traps in reference to the conduction and valence band edges.

Calculation of Trapped Charge in Poisson's Equation

The total charge caused by the presence of traps is subtracted from the right hand side of Poisson's equation. The total charge value is defined by:

$$Q_T = q(N_{tD}^{+} - N_{tA}^{-}) \quad \text{3-61}$$

where N_{tD}^{+} and N_{tA}^{-} are the densities of ionized donor-like and acceptor-like traps respectively. The ionized density depends upon the trap density, DENSITY, and its probability of ionization, F_{tA} and F_{tD}. For donor-like and acceptor-like traps respectively, the ionized densities are calculated by the equations:

$$N_{tD}^{+} = \text{DENSITY} \times F_{tD} \quad \text{3-62}$$

$$N_{tA}^{-} = \text{DENSITY} \times F_{tA} \quad \text{3-63}$$

In the case where multiple traps at multiple trap energy levels are defined the total charge becomes:

$$N_{tD}^{+} = \sum_{\alpha=1}^{k} N_{tD\alpha}^{+} \quad , N_{tA}^{-} = \sum_{\beta=1}^{m} N_{tA\beta}^{-} \qquad \text{3-64}$$

where k is the number of donor-like traps and m is the number of acceptor-like traps.

The probability of ionization assumes that the capture cross sections are constant for all energies in a given band and follows the analysis developed by Simmons and Taylor [254]. The probability of ionization is given by the following equations for acceptor and donor-like traps.

$$F_{tA} = \frac{v_n \mathtt{SIGN}\, n + e_{pA}}{v_n \mathtt{SIGN}\, n + v_p \mathtt{SIGP}\, p + e_{nA} + e_{pA}} \qquad \text{3-65}$$

$$F_{tD} = \frac{v_p \mathtt{SIGP}\, p + e_{nD}}{v_n \mathtt{SIGN}\, n + v_p \mathtt{SIGP}\, p + e_{nD} + e_{pD}} \qquad \text{3-66}$$

where SIGN and SIGP are the carrier capture cross sections for electrons and holes respectively, v_n and v_p are the thermal velocities for electrons and holes. For donor like traps, the electron and hole emission rates, e_{nD} and e_{pD}, are defined by:

$$e_{nD} = \frac{1}{\mathtt{DEGEN.FAC}}\, v_n\, \mathtt{SIGN}\, n_i exp\frac{E_t - E_i}{kT_L} \qquad \text{3-67}$$

$$e_{pD} = \mathtt{DEGEN.FAC}\, v_p\, \mathtt{SIGP}\, n_i exp\frac{E_i - E_t}{kT_L} \qquad \text{3-68}$$

where E_i is the intrinsic Fermi level position, E_t is the trap energy level as defined by E.LEVEL and DEGEN.FAC is the degeneracy factor of the trap center. The latter term takes into account that spin degeneracy will exist, that is the “empty” and “filled” conditions of a defect will normally have different spin and orbital degeneracy choices. For acceptor like traps, the electron and hole emission rates, e_{nA} and e_{pA}, are defined by:

$$e_{nA} = \mathtt{DEGEN.FAC}\, v_n\, \mathtt{SIGN}\, n_i \exp\frac{E_t - E_i}{kT_L} \qquad \text{3-69}$$

$$e_{pA} = \frac{1}{\mathtt{DEGEN.FAC}}\, v_p\, \mathtt{SIGP}\, n_i exp\frac{E_i - E_t}{kT_L} \qquad \text{3-70}$$

Table 3-7 User-Specifiable Parameters for Equations 3-62 to 3-68		
Statement	**Parameter**	**Units**
TRAP	E.LEVEL	eV
TRAP	DENSITY	cm^{-3}
TRAP	DEGEN.FAC	
TRAP	SIGN	cm^2
TRAP	SIGP	cm^2

Trap Implementation into Recombination Models

To maintain self-consistency, you need to take into account that electrons are being emitted or captured by the donor and acceptor-like traps. Therefore, the concentration of carriers will be affected. This is accounted for by modifying the recombination rate in the carrier continuity equations.

The standard SRH recombination term (see "Shockley-Read-Hall (SRH) Recombination" on page 197) is modified as follows:

$$R = \sum_{\alpha=1}^{l} R_{D_\alpha} + \sum_{\beta=1}^{m} R_{A_\beta} \quad \text{3-71}$$

where l is the number of donor-like traps, m is the number of acceptor-like traps. For donor-like traps, the function R is:

$$R_{D\alpha} = \frac{pn - n_{ie}^2}{\mathrm{TAUN}\left[p + \mathrm{DEGEN.FAC}\, n_{ie} exp\left(\frac{E_i - E_t}{kT_L}\right)\right] + \mathrm{TAUP}\left[n + \frac{1}{\mathrm{DEGEN.FAC}}\, n_{ie} exp\left(\frac{E_t - E_i}{kT_L}\right)\right]} \quad \text{3-72}$$

For acceptor like traps the function R is:

$$R_{A\beta} = \frac{pn - n_{ie}^2}{\mathrm{TAUN}\left[p + \frac{1}{\mathrm{DEGEN.FAC}} n_{ie} exp\left(\frac{E_i - E_t}{kT_L}\right)\right] + \mathrm{TAUP}\left[n + \mathrm{DEGEN.FAC}\, n_{ie} exp\left(\frac{E_t - E_i}{kT_L}\right)\right]} \quad \text{3-73}$$

The electron and hole lifetimes TAUN and TAUP are related to the carrier capture cross sections SIGN and SIGP through the equations:

$$\mathrm{TAUN} = \frac{1}{\mathrm{SIGN}\ v_n \mathrm{DENSITY}} \quad \text{3-74}$$

$$\mathrm{TAUP} = \frac{1}{\mathrm{SIGP}\ v_p\ \mathrm{DENSITY}} \quad \text{3-75}$$

The thermal velocities v_n and v_p are calculated from the following electron and hole effective masses.

$$v_n = \left(\frac{3kT}{m_n m_0}\right)^{1/2} \quad \text{3-76}$$

$$v_p = \left(\frac{3kT}{m_p m_0}\right)^{1/2} \quad \text{3-77}$$

To specify the effective masses directly, use the M.VTHN and M.VTHP parameters from the MATERIAL statement. If M.VTHN or M.VTHP or both are not specified, the density of states effective mass is extracted from the density of states (N_c or N_v) using Equations 3-31 and 3-32. In the case of silicon if M.VTHN or M.VTHP are not specified, the effective masses are calculated from:

$$m_n = 1.045 + 4.5 \times 10^{-4} T \quad \text{3-78}$$

$$m_p = 0.523 + 1.4 \times 10^{-3} T - 1.48 \times 10^{-6} T^2 \quad \text{3-79}$$

where T is the lattice temperature.

Table 3-8 User-Specifiable Parameters for Equations 3-72-3-75

Statement	Parameter	Units
TRAP	TAUN	s
TRAP	TAUP	s

The TRAP statement activates the model and is used to:

- Specify the trap type DONOR or ACCEPTOR
- Specify the energy level E.LEVEL parameter
- Specify the density of the trap centers DENSITY
- Specify the degeneracy factor DEGEN.FAC
- Specify either the cross sections, SIGN and SIGP, or the electron and hole lifetimes TAUN and TAUP.